

Gauge fields emerging from time reversal symmetry breaking for spin-5/2 fermions in a honeycomb lattice

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We propose an experimentally feasible setup with ultracold alkaline earth atoms to simulate the dynamics of U(1) lattice gauge theories in 2+1 dimensions with a Chern-Simons term. To this end we consider the ground state properties of spin-5/2 alkaline earth fermions in a honeycomb lattice. We use the Gutzwiller projected variational approach in the strongly repulsive regime in the case of filling 1/6. The ground state of the system is a chiral spin liquid state with $2\pi/3$ flux per plaquette, which spontaneously violates time reversal invariance. We demonstrate that due to the breaking of time reversal symmetry the system exhibits quantum Hall effect and chiral edge states. We relate the experimentally accessible spin fluctuations to the emerging gauge field dynamics. We discuss also properties of the lowest energy competing orders.

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One of the main motivations of studying ultracold atoms in optical lattices is the high extent of experimental control. Such systems are very flexible and therefore are good candidates for simulating other quantum systems, where experimental control is more cumbersome. There is a vast number of proposals where ultracold quantum gases can serve as simulators of condensed matter, or even high energy physics systems (see for instance Ref. [1]). An important example of such proposals concerns the recent experimental realization of trapping and cooling of ultracold alkaline earth atoms [2–4], which could serve for quantum simulators of high symmetry magnetism [5]. Despite of these spectacular developments, one of the most important goals of quantum simulators remains still to be realized, namely the simulation of quantum gauge theories, which appear first of all in high energy physics, but arise naturally also in many areas of condensed matter physics, such as physics of frustrated systems, or of high temperature superconductors [6]. The main difficulty here is to map the many modes of the gauge field to those of an atomic ensemble. Very recent proposals use mixtures of fermionic and bosonic atoms, so that the bosons are the mediators of the gauge field [7, 8].

Here we propose another, somewhat simpler, scheme with only a single species of ultracold atoms to simulate a 2+1 dimensional U(1) lattice gauge theory with a Chern-Simons term. Our proposal is based on the observation that low energy excitations of certain Mott insulators can be described by lattice gauge theories [6, 9]. The Mott insulator we consider here is formed by spin-5/2 alkaline earth atoms, such as ^{173}Yb , which, as was shown by Hermele *et al.* [10], can exhibit time reversal symmetry breaking, and have a so called chiral spin liquid (CSL) ground state in a square lattice. CSL states lack any kind of long range order, but due to the violation of time reversal invariance, they are stable also at low temperatures. The fluctuations above the CSL state are described by

a U(1) gauge theory with a Chern-Simons term arising from the chiral (time reversal symmetry breaking) nature of the ground state [11]. Here we treat the case of a honeycomb lattice; we show that the lowest energy spin liquid ansatz with one particle per site that respects the underlying lattice symmetries is a CSL. We describe also two other lowest energy spin liquid states, that can be stabilized in certain situations. We show also how the dynamics of the emerging gauge fields is measurable by spin correlation functions. Obviously, further motivation to study spin liquid phases in a honeycomb lattice with ultracold atoms is due to a newly rising interest in related challenging problems, like superconductivity in graphene [12–15], or other forms of time reversal symmetry breaking that appear for honeycomb and pyrochlore lattices [16, 17].

The main advantage of using alkaline earth atoms is that the nuclear spin I decouples from the angular momentum of the electrons J , which is zero in the ground state, and hence collision processes become spin independent. Therefore spin- I isotopes of alkaline earth atoms can be described to a very good accuracy by SU(N) symmetric model Hamiltonians, where $N = 2I + 1$, and we take $I = 5/2$, which is realized e.g. by ^{173}Yb . In an optical lattice the SU(N) symmetric Hubbard Hamiltonian takes the form

$$H = -t \sum_{\langle i,j \rangle, \alpha} \left(c_{i\alpha}^\dagger c_{j\alpha} + \text{H.c.} \right) + \frac{U}{2} \sum_{i, \alpha, \beta} c_{i\alpha}^\dagger c_{i\beta}^\dagger c_{i\beta} c_{i\alpha}, \quad (1)$$

where $c_{i\alpha}$ annihilates an atom at site i with spin $\alpha \in \{-\frac{5}{2}, \dots, \frac{5}{2}\}$, t stands for the tunneling amplitude, and U for the strength of the on-site interaction.

In the strongly repulsive regime, $U \gg t$, the motional (charge) degree of freedom of the fermions gets frozen at low temperatures leading to a Mott insulator state, and the system can be described by an effective SU(6) spin Hamiltonian [5, 9]. The ground state of such a Hamiltonian can be a Néel antiferromagnetic state with long

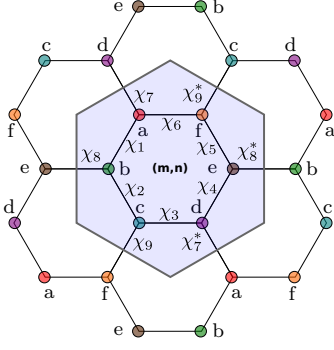


FIG. 1: (Color online) The unit cell for the mean-field approximation.

range order, or a spin liquid state without any kind of long range order [18] that can be described using the (resonating) valence bond concept [6, 19–21]. Hermele *et al.* have shown that the Néel order is ruled out by energy constraints for $SU(N)$ Hamiltonians for $N \geq 3$ [10].

Deeply in the Mott insulator region ($U \gg t$) and for $1/6$ filling, there is exactly one particle per site. From experimental point of view this is an appealing setup, in which undesired 3-body losses can be neglected. In this case particle tunneling is forbidden due to the very high energy cost of the multiply occupied sites. Only virtual hopping is allowed, and the Hamiltonian (1) can be approximated by

$$H_{\text{eff}} = g \sum_{\langle i,j \rangle, \alpha, \beta} c_{i\alpha}^\dagger c_{j\alpha} c_{j\beta}^\dagger c_{i\beta}, \quad (2)$$

with $g = -4t^2/U$. This effective Hamiltonian acts in the restricted Hilbert space of 1 atom per site; this condition is enforced by the local constraints: $\sum_\alpha c_{i\alpha}^\dagger c_{i\alpha} = 1$. The Hamiltonian (2) already exhibits local $U(1)$ gauge invariance, since it is invariant under the transformation $c_{i\alpha} \rightarrow c_{i\alpha} e^{i\theta_i}$, in accordance with the local constraints.

To study the ground state properties and the low energy excitations of the system we decouple the quartic terms via a mean-field treatment by introducing the average of the pair-correlation defined as

$$\chi_{ij} \equiv \sum_\alpha \langle c_{i\alpha}^\dagger c_{j\alpha} \rangle = \chi_{ji}^*. \quad (3)$$

The effective Hamiltonian takes then the mean-field form

$$H_{\text{mf}} = g \sum_{\langle i,j \rangle} \left[\sum_\alpha \left(\chi_{ij} c_{j\alpha}^\dagger c_{i\alpha} + \chi_{ji} c_{i\alpha}^\dagger c_{j\alpha} \right) - |\chi_{ij}|^2 \right]. \quad (4)$$

Though the mean-field Hamiltonian Eq. (4) is already quadratic, one still needs to make further assumptions about the solution in order to obtain a tractable set of equations. We choose a hexagonal unit cell containing 6 lattice sites, as depicted in Fig. 1; such cell respects the original lattice symmetries, and contains as many sites

as needed to form a $SU(6)$ singlet. As a consequence 9 independent mean-field amplitudes arise: $\chi_1 \dots \chi_9$, and the description through the Hamiltonian (4) inherently describes 6 bands inside the Brillouin zone. With the introduction of 6 Lagrange multipliers (one for each site of the unit cell) the local constraints can be enforced, and then the Mott insulator state with 1 particle per site is simply achieved by filling the lowest band.

By diagonalizing the Hamiltonian (4) one obtains the ground state $|\Psi^{\chi_{ij}}\rangle$; using then the self-consistency condition (3), one arrives at a set of equations for the mean-field amplitudes and for the local Lagrange multipliers. This set of equations is highly nonlinear and has several solutions. Because of the local $U(1)$ gauge structure, solutions related to each other by the transformation

$$\chi_{ij} \rightarrow \chi_{ij} e^{i(\theta_i - \theta_j)} \quad (5)$$

are equivalent, and have the same energy and the same physical spin wave function, obtained by the Gutzwiller projection, i.e., by restricting the solution to the space with one particle per site:

$$\Psi(\alpha_1, \alpha_2 \dots \alpha_m) = \langle 0 | \prod_i c_{i\alpha_i} | \Psi^{\chi_{ij}} \rangle. \quad (6)$$

The Wilson loop $\Pi_i = \prod_{\mathcal{P}_i} \chi_{ij}$ calculated for each plaquette \mathcal{P}_i is invariant under such transformations, and therefore is the same for gauge equivalent solutions. Note that due to our construction there are 3 nonequivalent plaquettes that can be considered as a 3 sublattice ansatz on the dual lattice: the triangular lattice formed by the plaquettes. Table I shows the three lowest energy mean-field solutions. The ground state solutions (first two lines of Table I) correspond to $\chi_1 = \chi_2 \dots = \chi_6 = r e^{\pm i\varphi}$ and $\chi_7 = \chi_8 = \chi_9 = r$, with $r \approx 0.82651$ and $\varphi = 2\pi/9$. The corresponding Wilson loops are $\Pi_i = r^6 e^{\pm i\Phi}$, with $\Phi = 2\pi/3$ flux. Therefore the ground state breaks time reversal invariance, and is a CSL state. Due to the violation of time reversal symmetry there is a double degeneracy in addition to the gauge structure. A higher energy staggered like phase is the next-lowest lying quasi-plaquette state that has a triple degeneracy with an energy of $E = -6.062$, as it is shown in the following 3 lines of Table I. This phase is the honeycomb analog of the (staggered) π -flux state of spin-1/2 fermions on a rectangular lattice, which is the lowest energy spin-liquid state for the non-doped Mott insulator. In our case, due to the frustrated nature of the dual lattice, the staggered flux phase is not energetically favorable. In this state the fluxes do not alternate sign, but they change between 0 and π in a way that every zero flux plaquette is surrounded by plaquettes with π fluxes. The last three lines of Table I show a valence bond crystal type ordering, where there is no flux threading through the disconnected plaquettes. This state is similar to the ground state of e.g. the spin-3/2 fermions in the square lattice at quarter filling [22]. This valence bond crystal also has a triple degeneracy. Figure 2 illustrates these three lowest energy states.

E	Π_1	Π_2	Π_3
-6.148	$-0.159 - 0.276i$	$-0.159 - 0.276i$	$-0.159 - 0.276i$
-6.148	$-0.159 + 0.276i$	$-0.159 + 0.276i$	$-0.159 + 0.276i$
-6.062	0.460	-0.223	-0.223
-6.062	-0.223	0.460	-0.223
-6.062	-0.223	-0.223	0.460
-6	1	0	0
-6	0	1	0
-6	0	0	1

TABLE I: Mean-field solutions. The first column represents the energy of the mean-field solution, the other three columns give the Wilson loops of the 3 different plaquettes.

In the CSL state the mean-field generated fluxes penetrating the plaquettes are analogous to those created by a magnetic field. As a consequence, quantum Hall effect can be observed. It is entirely generated in this case spontaneously by the mean-fields. It leads to appearance of chiral edge states, i.e. current carrying states localized at the boundaries in such a way that the opposite directions are separated to opposite edges. Figure 3 depicts the energy spectrum with the bulk bands and the edge states. For 1/6 filling only the lowest bulk band is filled, which is well separated from the next band. We have calculated the Chern number (C), which characterizes the quantum Hall effect by giving the number of counter propagating edge state pairs inside a bulk energy gap. We have found that $C = 6$ for the lowest gap, which

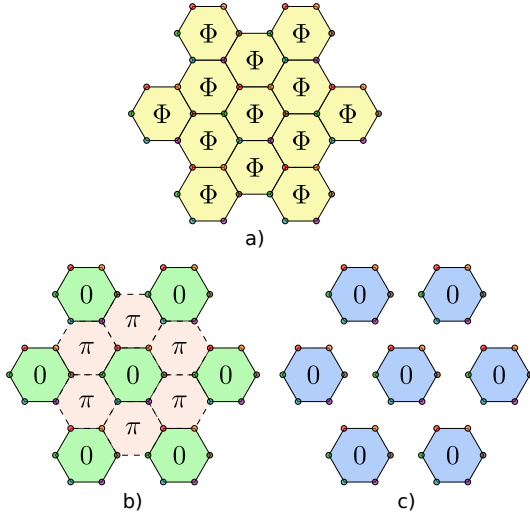


FIG. 2: (Color online) Lowest energy mean-field solutions. Subfigure a) illustrates the chiral spin-liquid configuration with all bonds having the same magnitude. Subfigure b) depicts the quasi-plaquette phase with real Wilson loops. The dashed line represents a smaller bond value than the solid line. Subfigure c) shows the plaquette phase configuration with only one nonzero Wilson loop per three cells. Links with a zero mean-field value are removed from the figure.

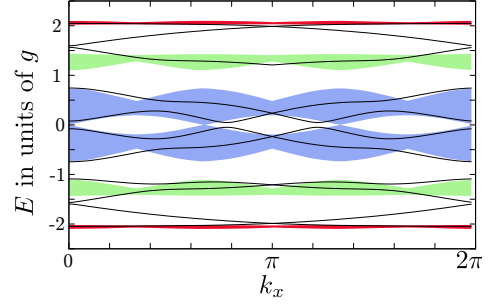


FIG. 3: (Color online) The energy spectrum of the system for open boundary conditions in one direction.

is in accordance with the observation that there is one edge state pair per spin component. It follows that an elementary flux of $\Phi_0 = \pi/3$ is attached to every spinon (the fractionalized quasi-particle excitation, created by the operators $c_{i,\alpha}^\dagger$), which in effect renders their statistics to an anyonic one. On the other hand it provides explanation for the $\Phi = 2\pi/3$ flux per plaquette of the ground state: since each site belongs to 3 plaquettes, every plaquette contains 2 spinons leading to $\Phi = 2\Phi_0$, as expected.

The low-energy fluctuations of the mean-field theory are given by the phase fluctuations of the mean-field amplitude, $\chi_{ij} = \chi_{ij}^{\text{mf}} e^{ia_{ij}}$, and by the lowest energy spinon excitations. The mean-field phase fluctuation a_{ij} is a gauge field with the transformation property $a_{ij} \rightarrow a_{ij} + \theta_i - \theta_j$. The low energy spinon excitations are coming from the vicinity of the energy maxima of the valence band, and from the energy minima of the conduction band. Since there are 6 such points, the low-energy dynamics is governed by spinons with 6 flavors interacting with a U(1) gauge field. By integrating out the high energy (gapped) spinon fields the resulting low energy theory is described by the following Lagrangian density in the continuum limit:

$$\mathcal{L} = \frac{1}{8\pi q^2}(\mathbf{e}^2 - vb^2) - \frac{C}{4\pi}\epsilon^{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda + \sum_{l=1}^6 \left[-ic_{l,\alpha}^\dagger(\partial_t - ia_0)c_{l,\alpha} + \frac{1}{2m_s}c_{l,\alpha}^\dagger(\partial_i + ia_i)^2c_{l,\alpha} \right], \quad (7)$$

where the constant q^2 arises from the integration of the spinon fields and is in the order of the spinon gap g . The fields \mathbf{e} , and b , are the artificial electric and magnetic fields, respectively, obtained from the scalar and vector potentials a_0 and a_i in the usual way. The constant $C = 6$ is the Chern number, and the speed of sound v is proportional to $1/g \sim U/t^2$. In the spinon part of the Lagrangian m_s stands for the effective mass of the spinons, which can be obtained from the curvature of the spinon dispersion around the 6 minimas. Due to the Chern-Simons term, the gauge bosons mediate only

a short range interaction between the spinons, and the mean-field solution is stable [9]. Therefore, the low energy properties of the system can be characterized by U(1) gauge field coupled to the spinons as matter fields. The corresponding gauge theory described by the Lagrangian (7) can be thus simulated with ultracold spin-5/2 fermions loaded into hexagonal lattice.

Ultracold alkaline earth atoms are produced routinely nowadays. A honeycomb optical lattice can also be created by sophisticated laser configurations [23]. Another, even cleaner experimental implementation would be to use the holographic methods of Greiner *et al.*, or Esslinger *et al.*, where an arbitrary two dimensional lattice potential can be created with the help of an optical imaging system [24, 25]. Detecting the CSL phase, or the emerging dynamical gauge theory is not straightforward, but possible. For example, one can measure nearest neighbor pair correlations [26], but there is only access to $|\chi_{ij}|$. In fact, according to the Elitzur's theorem non gauge invariant quantities, such as χ_{ij} , average to zero [27, 28]. A gauge invariant quantity sensitive to chirality and possible to measure is the phase of a loop, which can be detected directly by measuring 3-spin correlations: $\vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$. It's nonzero value witnesses for the chiral nature of the spin liquid phase [11]. Finally, and more importantly, one can measure in experiments, using for instance spin polarization spectroscopy [29], the spin structure factor $S^{zz}(i, j; t) = \langle S_i^z(t) S_j^z(0) \rangle$ at site i and j at time t and zero, respectively. This quantity can be expressed with the help of the four point spinon Green's functions, and in the RPA approximation is given by

$$S^{zz}(\mathbf{k}, \omega) = F_{\alpha\beta}^z F_{\beta\alpha}^z \frac{\Pi(\mathbf{k}, \omega)}{1 - 6 D(\mathbf{k}, \omega) \Pi(\mathbf{k}, \omega)}, \quad (8)$$

with $F_{\alpha\beta}^z$ being the z -component of the spin matrix in the 5/2 representation. The quantity $\Pi(\mathbf{k}, \omega)$ is the spinon polarization function, which to lowest order is simply the contribution of the bubble diagram, and $D(\mathbf{k}, \omega)$ is the photon propagator up to a numeric matrix for contracting the space time indices. Due to the hybridization of the gauge field and spinon propagators one can find resonances in the magnetic response function (8) belonging to the spinon and to the gauge field excitations. Therefore magnetic response measurements are suitable to reveal the gauge structure of low-lying excitations, and the chiral nature of the ground state.

We have studied the one particle per site Mott insulator phases of spin-5/2 ultracold alkaline earth atoms in the honeycomb lattice. We have found that the ground state is a chiral spin liquid state with broken time reversal symmetry. Thanks to the finite gap appearing in the spinon spectrum, we have integrated out the high energy spinon fields and arrived to a dynamical U(1) gauge field theory with a Chern-Simons term. This gauge theory describes the spin fluctuations of the system, and therefore the gauge field dynamics can be accessed experimentally with the help of spin response measurements.

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